Title:	Assembly Operations Welding Filter(s) in Drum Calculation
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1.0 INITIATION

1.1 Calculation Status:	Preliminary ☐	Final ☒

1.2 DCF No.: N/A	DCF Title: N/A

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1.4 Superseded Calculation No.: N/A

1.5 Facility Name(s): TA-55	1.6 Organization: NPI-6
1.7 Structure/ System ID: SCNTR	1.8 Structure/ System Name: Containers for movement of SNM OS GBs
1.9 Component ID: CONT-7A55GAL	1.10 Component Name: DOT Type A 55GAL Drum

1.11 Structure, System, or Component Nuclear Functional Classification

SC ☐   SS ☒   OHC ☐   NS ☐   N/A ☐

1.12 Structure, System, or Component Management Level

ML-1 ☐   ML-2 ☒   ML-3 ☐   ML-4 ☐   N/A ☐

If "N/A" is checked then explain: Calculation

1.13 Associated with Technical Baseline:	Yes ☒	No ☐

1.14 Is Cover Sheet being used to document a calculation from an external organization?   Yes ☐   No ☒

If yes, mark "N/A" in Field 3.2 Verifier and add description below.

Description:

2.0 SECURITY CLASSIFICATION REVIEW

2.1 Security Classification: Unclassified

2.2 DC/RO: *(Name, Z Number, Organization, Signature, Date)*

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3.0 APPROVALS

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3.4 FDAR: *(Name, Z Number, Organization, Signature, Date)*

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4.0 REGISTERED PROFESSIONAL ENGINEER SEAL:

5.0 REVISIONS						
Rev	Date	Description of Change(s)	Preparer	Verifier	RM	FDAR
0		Original Issue				

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1.0   PURPOSE

This calculation documents the estimation of temperature and pressure rise inside a 55-gal TRU waste drum with a HEPA filter containing Titanium and Tantalum fume dust based on operational history.

On 2/26/2021 an energy release event occurred during waste bagout. Two bagged HEPA filters (one standing open-face media up) and a spacer were in the drum. The bags may have preserved an inert Argon atmosphere around the filters. An empty, lidless con-flat container was dropped onto the filter media. This caused a loud noise and a quick shower of sparks, reddish orange in color. The HEPA filters in question were the Flanders 8" inch diameter, 5.875" depth, silica media, nuclear grade HEPA filters, stainless steel clad type, and model number is 0-007-D-43-R0-Nu-00-00-Z93555H. The estimated HEPA filter weight is 5 to 7 lb. The PS code was AO (Assembly Operation). The filter media of HEPAs was very dark in color.

The initial investigation found there were very low Rad materials on the filters. It was conjectured that dropping the con-flat container onto the bagged filters violated the bags, allowing oxygen into the filters, and added energy to the system. This caused rapid oxidation of Titanium and Tantalum fume dust collected on the HEPA filter from laser welding process.

This calculation estimates the possible maximum pressure rise caused by the rapid oxidation of Titanium and Tantalum fume dust collected on one HEPA filter.

2.0   METHODOLOGY

The possible Titanium and Tantalum fume dust loading on the HEPA filter was estimated based on the welding process (Ref. 6). The estimated masses of Titanium and Tantalum are listed in Table 1.

Table 1. Calculated masses of Ti and Ta on HEPA filters

Filter Change Date	2/19/2021	6/26/2020	1/18/2020	10/15/2019	2/10/2019	9/18/2018
Calculated mass of Ti fume, g	0.64	1.25	0.52	3.54	1.6	0.33
Calculated mass of Ta fume, g	0.08	0	0	0.01	0	0.18

The oxidation of Titanium and Tantalum can be described by the following equations:

$$Ti + \ O_2 \rightarrow TiO_2$$

$$4\,Ta + \ 5\,O_2 \rightarrow 2\,Ta_2O_5$$

The enthalpy of these reactions is calculated. Then the pressure rise of the drum is calculated based on the energy released if these Titanium and Tantalum were rapidly oxidized at the same

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time. The maximum amount of these metals that could be on a filter without over pressurizing a drum is also calculated.

3.0   ACCEPTANCE CRITERIA

N/A

There are no explicit acceptance criteria for this calculation.

4.0   UNVERIFIED ASSUMPTIONS

N/A.

5.0   ASSUMPTIONS

5.1   The weight of Flanders 8" diameter nuclear grade HEPA filter is about 5 to 7 lbs. The filter media is boron silicate fiber glass (https://www.aafintl.com/en/commercial/browse-products/commercial/hepa-ulpa-filters/hepa---nuclear-grade) . 5 lbs (2270 g) weight is utilized in the calculation. This assumption is conservative. (Ref. 5)

5.2   Use the specific heat capacity of silicon dioxide (SiO_2), 0.740 J/g.K, as the specific heat capacity of HEPA filter. Specific heat capacity of boron silicate fiber glass isn't listed on CRC handbook. On wikipedia (https://en.wikipedia.org/wiki/Borosilicate_glass), the specific heat of borosilicate glass is listed as 0.83 J/g.K. Since 0.740 J/g.k is less than 0.83 J/g.k. Delta T is inversely proportional to this number, so the smaller value the more conservative. This assumption is conservative.

5.3   Initial temperature is 298 K (25 °C).

5.4   Initial pressure is 11.2 psia (0.76 atm), the atmosphere pressure at Los Alamos.

5.5   The drum is adiabatic (heat loss is neglected). This assumption is conservative.

5.6   The drum is airtight (no gas loss). Therefore the volume of the air inside waste drum remains constant. . This assumption is conservative.

5.7   Use the isochoric specific heat of air at 298 K, C_v = 20.78 J/mol.K in the calculation. Since the drum filter can vent and isochoric specific heat is lower than isobaric specific heat, this assumption is conservative.

5.8   Ideal gas law applies.

5.9   Titanium dioxide (TiO_2) and Ta_2O_5 are oxidation products. Titanium can form other suboxides such as TiO, Ti_2O_3 and Ti_3O_5 before it forms TiO_2. Even though the enthalpy of formation of Ti suboxides are high, the energy per mole of Ti will be less. TiO_2 is the highest bound oxide.

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6.0   LIMITATIONS

N/A

7.0   CALCULATION INPUTS

CRC Handbook and Tables of Thermal Properties of Gases were used to obtain the required thermal properties of air and silicon dioxide. CRC Handbook and Jacob et al (2009) were used to obtain enthalpy values for the reactions.

8.0   COMPUTER HARDWARE AND SOFTWARE

N/A

9.0   SUMMARY AND CONCLUSIONS

Based on the estimation of Titanium and Tantalum mass (Table 1), assuming the drum has one HEPA filter inside, the rapid oxidation of Titanium and Tantalum on HEPA filters will cause maximum 39 K temperature increase and 1.5 psig pressure increase. The pressure increase is less than than the 14 psig seal failure value from DOE STD 5506-2007. Since the final temperatures are all below 100 ^{o}C, there is a low risk to initiate combustion reaction of cheese cloth and plastic inside the drum. The void volume inside the drum has little impact on the calculated temperature and pressure. This is due to the fact that HEPA filters absorb more heat than air does and the volume of air inside has less impact than the weight of HEPA filter has.

Assuming the drum is filled, has 104 L void volume, has one HEPA filter inside, and neglecting the heat absorption of other materials inside drum, 33.00 g Titanium is the maximum amount on the filter without over-pressurizing the drum; 115.59 g Tantalum is the maximum amount on the filter without over-pressurizing the drum.

The following are related temperature and pressure limits for TRU waste drum.

- DOE-STD-5506-2007 states seal failure occurs at about 14 psig.
- According to DOE-STD-5506-2007, 28 psig is the pressure to cause lid loss in a rapidly rising catastrophic physical ejection during a fire event.

For TRU waste drum containing combustible materials, document C-CDE-17-001 (Ref. 7) highlights an experimental analysis that was done to characterize the temperature at which cheesecloth, ignites. The conclusion was that the onset of mass loss of untreated cheesecloth occurred at 82 ^{o}C to 313 ^{o}C.

Compared to the above limits, the calculated temperature and pressure in this calculation are much less.

Since the calculation neglects the heat absorption of other materials inside the drum, the heat loss, the latent heat of melting of metals and plastic, and gas release through the filter, the calculation is conservative.

10.0   REFERENCES

1.   CRC handbook of chemistry and physics: a ready-reference book of chemical and physical data. Haynes, W. M.; Lide, David R. 2011

2.   DOE-STD-5506-2007. Preparation of Safety Basis Documents for Transuranic (TRU) Waste Facilities.
3.   Jacob et al. An update on the thermodynamics of Ta_2O_5. J. Chem. Thermodynamics 41 (2009) 748–753.
4.   P409-1, LANL Waste Acceptance Criteria
5.   23_4233_19 Auxiliary Nuclear Grade HEPA filters.
6.   CAL-21-TA55-IPGW-035-D. Determination of fume generation during conduction mode Yb-fiber laser welding of titanium and tantalum
7.   C-CED-17-001. Effect of Cheesecloth Exposure to 15.6M Nitric Acid and Elevated Temperature with TGA/DCS/MS Analysis
8.   NIST webpage for thermochemical data. https://webbook.nist.gov/cgi/cbook.cgi?ID=C1317802&Units=SI&Mask=2#Thermo-Condensed

11.0   CALCULATION

11.1   **Assume drum only has one HEPA filter**

Assume a 55-gallon (208 L) drum only has one Flanders 8-inch HEPA round filter inside. It is unlikely that a drum will contain solely one HEPA filter, however there is no known, consistent proportion of the drum volume occupied with other waste. Therefore for simplicity this calculation assumes the 208 L is occupied by air and one 8-inch HEPA round filter. The packing volume of the 8-inch round HEPA filter is 4.84 L. However, the filter media is porous. Therefore, the real material volume of the HEPA filter is much less than 4.84L. In this case, the volume of the HEPA filter is negligible in the calculation.

1.   Enthalpy of reactions

       According to CRC handbook and Jacob et al., at 298 K, the enthalpy of formation of TiO_2 is -944 kJ/mol and the enthalpy of formation of Ta_2O_5 is -2038 kJ/mol (exothermal reactions).

2.   Heat generated

       $Q = m_{Ti}$ g ÷ 47.87 g/mol X 944 kJ/mol + m_{Ta} ÷ 181 g/mol X 0.5 X 2038 kJ/mol

3.   Temperature increase

       The specific heat capacity of dry air is $C_{v, air}$ = 20.78 J/mol•K
       At standard condition (273 K, 1 atm), the volume of 1 mole air is 22.4 L.
       At 298 K and 7,300 feet elevation (0.76 atm) at Los Alamos, the volume of 1 mole air is 32.2 L.
       The number of moles of dry air in the drum is n=208/32.2 = 6.46 mol

       The specific heat capacity of a HEPA filter (silicon dioxide) is $C_{p, HEPA}$ = 0.740 J/g•K
       The mass of HEPA filter is m = 2270 g

       Temperature increase is
       $\Delta T = Q/(C_{p, HEPA} \cdot m + C_{p, air} \cdot n)$
       Final temperature T_2 = 298 + ΔT
       Final temperature in Celsius $T_{2,c}$ = T_2 - 273

4.   Pressure increase

Using ideal gas law

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$
$$V_1 = V_2$$
$$P_2 = \frac{P_1 T_2}{T_1}$$

The pressure increase is ΔP = P_2 - P_1

Table 2 lists the calculated results

Table 2 Calculated Temperature and Pressure for 208 L Void Volume in Drum

Filter Change Date	2/19/21	6/26/20	1/18/20	10/15/19	2/10/19	9/18/18
Calculated Temperature increase, K	7	14	6	38.5	17	4
Final Temperature, K	305	312	304	337	315	302
Final Temperature, Celsius	32	39	31	64	42	29
Calculated Pressure increase, psig	0.3	0.5	0.2	1.4	0.7	0.2

11.2   **Assume drum is filled and has one HEPA filter**

Assume 55-gallon (208 L) drum is filled and has one 8-inch round HEPA filter inside. Although the drum is filled, there are a lot of void spaces between the materials inside. The average empty volume (air volume) of the 9 containers that possible have HEPA filters is estimated based the weight of the material inside. The estimated void volume is 180 L. Assume only the HEPA filter and air absorb the heat released from Titanium and Tantalum oxidation, and neglect the heat absorption of other materials inside drum. Assume there is no other adverse reactions inside the drum.

1.   Enthalpy of reactions

Same as 11.1.

2.   Heat generated

Same as 11.1

3.   Temperature increase

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The number of moles of dry air in the drum is n = 180/32.2 = 5.59 mol

Temperature increase is
$\Delta T = Q/(C_{p, HEPA} \cdot m + C_{p, air} \cdot n)$
Final temperature $T_2 = 298 + \Delta T$
Final temperature in Celsius $T_{2,c} = T_2 - 273$

4.   Pressure increase

$$P_2 = \frac{P_1 T_2}{T_1}$$

The pressure increase is $\Delta P = P_2 - P$
Table 3 list the calculation results

Table 3 Calculated Temperature and Pressure for 180 L Void Volume in Drum

Filter Change Date	2/19/21	6/26/20	1/18/20	10/15/19	2/10/19	9/18/18
Calculated Temperature increase, K	7	14	6	39	18	4
Final Temperature, K	305	312	304	337	316	302
Final Temperature, Celsius	32	39	31	64	43	29
Calculated Pressure increase, psig	0.3	0.5	0.2	1.5	0.7	0.2

5.   The impact of void volume.
Comparison of Table 3 and Table 2 shows the difference between 208L results and 180 L results is minimal. This is due to the fact that HEPA filters absorb more heat than air does and the volume of air inside has less impact than the weight of HEPA filter has. Table 4 shows the calculated results of filter changed on 10/15/2019 at different void volume. The results are close.

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Table 4 Calculated Temperature and Pressure at different Void Volume

Filter Change Date	10/15/2019	10/15/2019	10/15/2019
Void Volume, L	**208**	**180**	**10**
Calculated Temperature increase, K	**38.5**	**39**	**41**
Final Temperature, K	**336.5**	**337**	**339**
Final Temperature, Celsius	**64**	**64**	**66**
Calculated Pressure increase, psig	**1.4**	**1.5**	**1.6**

11.3   The maximum amount of Ti or Ta that could be on a filter

The maximum amount of Titanium fume dust that could be on a filter without over pressurizing a drum is calculated based on 14 psig pressure rise inside 55-gallon drum. Assume the drum has 104 L void volume. This assumption is conservative. Assume only Titanium or Tantalum fume dust is on the HEPA filter.

1.   Pressure increase

The pressure increase is 14 psig.
The final pressure is $P_{2, max}$ = 14 + 11.2 = 25.2 psia

2.   Temperature increase
Using ideal gas law

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$
$$V_1 = V_2$$
$$T_2 = \frac{P_2 T_1}{P_1}$$

$T_{2, max}$ = (25.2 psia × 298 K)/11.2 psia = 671 K

ΔT_{max} = 671 – 298 = 373 K

3.   Heat Generated

Q_{max} = ΔT_{max} × ($C_{p, HEPA}$•m + $C_{v, air}$•n)
    = 373 K × (0.740 J/g•K ×2270 g + 20.78 J/mol•K ×3.23 mol)
    = 650726 J
    = 650.726 kJ

4.   Maximum amount of Titanium

The enthalpy of formation of TiO_2 is 944 kJ/mol.

The maximum amount of Ti is:

$M_{Ti,max}$ = Q_{max} ÷ 944 kJ/mol × 47.87 g/mol = 33.00 g

5.   Amount of Tantalum

The enthalpy of formation of Ta_2O_5 is 2038 kJ/mol.

The maximum amount of Ta is:

$M_{Ta,max}$ = Q_{max} ÷ 2038 kJ/mol × 2 ×181 g/mol = 115.59 g